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NUMERICAL INTEGRATION OF THE CONTINUITY EQUATIONS

Appendix D

of

Development of a Simulation Model
for Estimating Ground Level Concentrations
of Photochemical Pollutants

Prepared by

Systems Applications, Inc.
Beverly Hills, California 90212

for the

Air Pollution Control Office
of the Environmental Protection Agency
Durham, North Carolina 27701

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A variant of the method of fractional steps was adopted for this study; it is based on the repeated but separate solution of three two-dimensional problems--in (x,t), (y,t), and (z,t) space--at each time step. Experience indicates that the procedure (with second or fourth-order approximation included) is stable and poses no particular computational difficulties. The basis for the selection of the numerical technique adopted is discussed. A detailed exposition of the method is given. The discussion is concluded with an evaluation of the procedure and a summary of experience with its use.

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INTRODUCTION

The simulation model for estimating ground level concentrations of photochemical pollutants is based on the equations of continuity for a turbulent fluid in which chemical reactions occur. These equations are given by:

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial c_i}{\partial x}\right)$$

$$+ \frac{\partial}{\partial y}\left(K_y\frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c_i}{\partial z}\right) + R_i\left(c_1, c_2, \ldots, c_p\right) + S_i$$

$$i = 1,2,\ldots,p \qquad \text{(D-1)}$$

$$\text{for} \quad x_W \leq x \leq x_E$$
$$y_S \leq y \leq y_N$$
$$h(x,y) \leq z \leq H(x,y,t)$$
$$t \geq t_o$$

where
- x,y = horizontal coordinates
- z = vertical coordinate
- u,v,w = three components of average wind velocity vector
- c_i = time-averaged concentration of species i
- K_x, K_y, K_z = turbulent eddy diffusivities
- S_i = rate of emission of species i from elevated sources
- R_i = rate of production of species i through chemical reaction
- x_W, x_E, y_S, y_N = west, east, south, and north model boundaries respectively
- $h(x,y)$ = terrain elevation
- $H(x,y,t)$ = elevation of the inversion base

Assuming that turbulent diffusion in the x and y directions can be neglected, Equation (D-1) simplifies to:

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial z}\left(K_z\frac{\partial c_i}{\partial z}\right) + R_i + S_i \qquad \text{(D-2)}$$

$$i = 1,2,\ldots,p$$

The initial and boundary conditions are:

initial $$c_i(x,y,z,t_o) = f_i(x,y,z)$$

boundary (1) $$-K_z \frac{\partial c_i}{\partial z} = Q_i(x,y,t) \qquad \text{at } z = h(x,y)$$

(2) if $W \geq 0$, then $-K_z \frac{\partial c_i}{\partial z} = 0$

if $W < 0$, then $W\, g_i(x,y,z,t) = W\, c_i - K_z \frac{\partial c_i}{\partial z}$ at $z = H(x,y,t)$

where $W = w - u \frac{\partial H}{\partial x} - v \frac{\partial H}{\partial y} - \frac{\partial H}{\partial t}$

(3) $$c_i = g_i(x,y,z,t) \qquad \text{at } x = x_W \text{ (or } x_E) \quad y = y_S \text{ (or } y_N)$$

where x and y are at boundaries through which the prevailing winds enter.

and where $Q_i(x,y,t)$ = surface flux of species i
$f_i(x,y,z)$ = initial concentration distribution of species i
$g_i(x,y,z,t)$ = function expressing the concentration of species i on the boundary at points of inflow

These equations, which are a repetition of Equations (2) in the main text, are coupled since they share a common argument in the terms $R_i(c_1, c_2, \ldots, c_p)$. We are thus confronted with the problems of solving p coupled, nonlinear partial differential equations in four dimensional space (x,y,z,t).

Finite difference methods have enjoyed widespread use in the numerical integration of partial differential equations. In particular, they have been successfully applied in the solution of a variety of three dimensional (x,y,t) problems in fluid mechanics and diffusion. Unfortunately, however, there is a dearth of reported experience in the integration of more complex systems of equations, such as Equations (D-1). It was thus necessary to investigate the use of modified versions of techniques developed for simpler systems of equations.

The approach adopted for this study, a variant of the method of fractional steps, is based on the repeated but separate solution of three two-dimensional problems--in (x,t), (y,t), and (z,t) space--at each time step. The solution procedure is implicit and iterative in (z,t) space, explicit and direct in (x,t) and (y,t) space. The chemical reaction and source terms, R_i and S_i, are included in the (z,t) portion of the integration. Truncation errors incurred due to the finite difference

approximation have been examined in tests of second and fourth-order methods, as applied to the horizontal advective portions of the fractionated equations--the (x,t) and (y,t) problems. The fourth-order procedure appears to be significantly more accurate in treating horizontal advection. It is still unclear, however, whether inclusion of the higher-order approximation in the overall model is warranted since a second-order method is used in the vertical, or (z,t), portion of the calculations. Tests of the two approximations are continuing. Finally, our experience thus far indicates that the procedure (with second or fourth-order approximation included) is stable and poses no particular computational difficulties.

In Section I of this Appendix, we discuss the basis for the selection of the numerical technique adopted. A detailed exposition of the method is given in Section II. We conclude the discussion, in Section III, with an evaluation of the procedure and a summary of our experience to date with its use.

I. SELECTION OF A FINITE DIFFERENCE TECHNIQUE

Equations (D-2) have characteristics of both hyperbolic and parabolic equations. Many methods have been reported in the literature for the solution of these classes of equations. In evaluating available methods, one must consider the following characteristics of each:

a) stability

b) accuracy

c) computer storage requirements

d) computing time requirements--expressible as the ratio of computing time to simulation time.

e) ease of implementation-adaptability of the method to the solutions of Equations (D-2)

In this section we briefly examine several classes of finite difference methods with these criteria in mind.

Finite difference techniques are often classified as explicit or implicit, depending on whether each succeeding integration step is direct or is based on the simultaneous solution of difference equations. While implicit techniques are computationally more burdensome than explicit methods, they do offer the advantage of larger ranges over which they are stable. Other finite difference methods exist which are difficult to classify in this way. Typically, these techniques have the characteristics of implicit methods yet, because of some unique aspect of the particular technique, involve less burdensome calculations than are normally expected with an implicit method. Two such techniques were considered for use in the solution of Equations (D-2), the method of fractional steps and the method of alternating directions.

The numerical integration technique that was ultimately adopted was selected by elimination. The reasoning was as follows:

a) Classical implicit methods involve the inversion of extraordinarily large matrices when applied to Equations (D-2), matrices on the order of 25,000 in size for a grid of 25 x 25 x 10 with four coupled equations. Even with a grid of substantially fewer nodes, the computational times would be excessive.

b) Explicit schemes were ruled out because of the highly nonlinear nature of the reaction rate terms. When coupled reaction rate equations are solved for conditions under which chemical rate processes (and not transport processes) are limiting, and these equations are thus expressible as ordinary differential equations, special

methods must be employed in their solution to ensure stability (See Appendix B, Section IV). The need for such methods is, if anything, more pronounced in the treatment of the coupled, nonlinear partial differential equations.

c) The method of alternating directions was attractive, as it possesses the stability characteristics of classical implicit techniques and yet involves the manipulation and inversion of tridiagonal matrices. A major simplification and savings in computational time is thereby realized, when compared to classical implicit methods, (see Richtmyer and Morton (1967) for further details). Unfortunately, knowledge of the concentration distribution (25 x 25 x 10 x 4 values) at three levels of time (current and two previous) are required. In order to store this information, use of external memory would be required, resulting in extended computation times.

d) The method of fractional steps involves the fragmentation of an n dimensional partial differential equation (with time as a variable) into n-1 two-dimensional partial differential equations. An implicit formulation is commonly used for those fragments which are parabolic (i.e., contain second partials or diffusion terms), an explicit formulation for those which are hyperbolic, (i.e., advection only). Since diffusion is included only in the vertical, and since we consider a maximum of ten strata, the implicit portion does not constitute a particular computational burden (inversion of a 10 x 10 tridiagonal matrix).

The method of fractional steps thus appears to be preferable to other classes of techniques for the particular problem under consideration.

The method of fractional steps was developed in the Soviet Union in the late 1950's. Since difference equations can be written in several ways, a variety of formulations of this method have been developed (see Richtmyer and Morton (1967) for a list of references). We have adopted the Crank-Nicolson treatment for the (z,t) fragment and have considered both second and fourth-order difference methods given by Crowley (1968) and Fromm (1969) for the (x,t) and (y,t) fragments. In the next section we present details of these schemes.

II. THE METHOD OF FRACTIONAL STEPS AND ITS APPLICATION TO THE INTEGRATION OF THE CONTINUITY EQUATIONS

The problem under consideration is the numerical solution of Equations (D-2), six partial differential equations in three spatial dimensions and time, with advection in all three directions and diffusion only in the vertical, or z, direction. Four of the six equations are coupled through the reaction rate terms. In applying the method of fractional steps, we fragment the partial differential equation into three separate two-dimensional partial differential equations, in (z,t), (x,t), and (y,t), with the inclusion of the reaction and elevated source terms in the (z,t) fragment. The solution in (z,t) is implicit, while the solution in (x,t) and (y,t) is explicit. Each step in time is comprised of the solution of each of the three fragments of Equations (D-2). Before presenting the details of the method, however, we wish to discuss certain aspects of the equations and their solution.

Order of the Method

Both second and fourth-order finite difference approximations have been considered for the two horizontal integrations, in (x,t) and (y,t), in which only advection is included. A second-order scheme was selected for the (z,t) fragment, as a fourth-order approximation was not justifiable due to the limited resolution in the z direction. The advantage of a second-order method in (x,t) and (y,t) is that it involves less computation than a higher-order method, but at a price of reduced accuracy. As our experience with both second and fourth-order methods is not yet sufficient to have made a choice between them, we present both. See Section III, however, for a more detailed discussion relating our experience with these alternative formulations.

Transformation of the Governing Equations

In Appendix C we discussed at length the unique nature of the temperature inversion that is so often present over Los Angeles. One of its most notable features is an increase in elevation of the base of the inversion with distance from the coast. We wish to include this feature in our finite difference formulation of Equation (D-2), and at the same time specify the base of the inversion as the upper boundary of the airshed. Unfortunately, since ground elevation and the height of the inversion base vary with x, y and z, the region being modeled is not rectangular (in three dimensions). It is thus convenient to perform a change of variables to a coordinate system in which this region is rectangular. To do this, we set

$$\xi = \frac{x}{x_E - x_W} \qquad \text{(D-3a)}$$

$$\eta = \frac{y}{y_N - y_S} \qquad \text{(D-3b)}$$

$$\rho = \frac{z - h(x,y)}{H(x,y,t) - h(x,y)} \qquad \text{(D-3c)}$$

Under this change of variables, Equations (D-2) become

$$\frac{\partial c_i}{\partial t} + \frac{u}{x_E - x_W}\frac{\partial c_i}{\partial \xi} + \frac{v}{y_N - y_S}\frac{\partial c_i}{\partial \eta} + \frac{W}{\Delta H}\frac{\partial c_i}{\partial \rho} = \frac{1}{\Delta H^2}\frac{\partial}{\partial \rho}\left(K_\rho \frac{\partial c_i}{\partial \rho}\right)$$

$$+ R_i + S_i \qquad \text{for} \quad i = 1,2,\ldots,p \qquad \text{(D-4)}$$

where $\Delta H = H(x,y,t) - h(x,y)$

$$W = w - \frac{u}{x_E - x_W}\left(\frac{\partial h}{\partial \xi} + \rho\frac{\partial \Delta H}{\partial \xi}\right) - \frac{v}{y_N - y_S}\left(\frac{\partial h}{\partial \eta} + \rho\frac{\partial \Delta H}{\partial \eta}\right) - \rho\frac{\partial H}{\partial t}$$

for $t \geq t_o$
$0 \leq \xi \leq 1$
$0 \leq \eta \leq 1$
$0 \leq \rho \leq 1$

The initial and boundary conditions are:

initial $\quad c_i(\xi,\eta,\rho,t_o) = f_i(\xi,\eta,\rho)$

boundary (1) $\quad \frac{-K_\rho}{\Delta H}\frac{\partial c_i}{\partial \rho} = Q_i(\xi,\eta,t)$ $\quad$ at $\rho = 0$

(2) if $W \geq 0$, then $\frac{-K_\rho}{\Delta H}\frac{\partial c_i}{\partial \rho} = 0$ $\quad$ at $\rho = 1$

if $W < 0$, then $\quad Wg_i = Wc_i - \frac{K_\rho}{\Delta H}\frac{\partial c_i}{\partial \rho}$

(3) $\quad c_i = g_i(\xi,\eta,\rho,t)$ $\quad$ at $\xi = 0,(\xi = 1)$
$\eta = 0,(\eta = 1)$

where ξ and η are at boundaries through which the prevailing winds enter.

Henceforth, we will be concerned with the solution of Equations (D-4) in a rectangular grid with spacing $\Delta\xi$, $\Delta\eta$, and $\Delta\rho$. For a 25 x 25 x 10 grid, these values are 0.04, 0.04, and 0.1 respectively, independent of time.

Temporal Resolution

The temporal resolution is associated with the frequency with which the primary variables are altered. The resolution of available data is the determining factor. Wind speed and direction are reported hourly, air quality data are similarly reported, and the emissions data, based on the emissions inventory reported in Appendix A, also have a temporal resolution of one hour. It thus seemed appropriate to carry out calculations of the upper wind field, aircraft emissions, and power plant emissions only once an hour, rather than at every time step. This simplification necessitates fixing the height of the inversion base for a period of one hour, then instantaneously moving it to a new level (over each of 625 columns of air) where it remains fixed for the following hour.* A spline interpolation procedure is employed to redistribute the concentration field from the old grid to the new grid.

Nomenclature

Under the best of circumstances, the nomenclature associated with the exposition of a finite difference formulation is clumsy. Our application is no exception, and, in fact, is rather more burdensome than is common. With apologies, then, the concentration distribution on the grid is denoted by ${}^{m}_{\ell}C^{n}_{i,j,k}$

where ${}^{m}_{\ell}C^{n}_{i,j,k} = {}^{m}_{\ell}C[(i-\tfrac{1}{2})\Delta\xi, (j-\tfrac{1}{2})\Delta\eta, (k-\tfrac{1}{2})\Delta\rho, n\Delta t]$

and ℓ is an index denoting chemical species.

i,j,k are indices related to location in the ξ-η-ρ coordinate system.

n is an index in time.

m refers to the iteration number.

Returning now to a presentation of the procedure, we remind the reader that the calculation of ${}^{n+1}_{\ell}C_{i,j,k}$ given ${}^{n}_{\ell}C_{i,j,k}$ requires three steps:

* Computational considerations also affected the decision to adjust the inversion base at hourly intervals. The repetition of the upper wind field calculation at each time step would greatly increase computation time.

Step I: Integration in the ρ direction
Step II: Integration in the ξ direction
Step III: Integration in the η direction

We first present the calculations for the formulation in which a second-order approximation is applied in each of the three steps. We then give the equations for Steps II and III using the fourth-order formulation. As a second-order implicit calculation is carried out in the ρ (or z) direction in either case, Step I is unchanged.

Step I - Integration in the ρ direction

We advance ${}_{\ell}C^{n}_{i,j,k}$ to ${}_{\ell}C^{*}_{i,j,k}$ by the following iterative difference scheme:

$$\frac{{}_{\ell}{}^{m}C^{*}_{i,j,k} - {}_{\ell}C^{n}_{i,j,k}}{\Delta t} + \frac{W_{i,j,k}}{\Delta H^{n}_{i,j}} \left(\frac{{}_{\ell}{}^{m}C^{*}_{i,j,k+1} + {}_{\ell}C^{n}_{i,j,k+1} - {}_{\ell}{}^{m}C^{*}_{i,j,k-1} - {}_{\ell}C^{n}_{i,j,k-1}}{4\,\Delta\rho} \right)$$

$$= \frac{1}{2(\Delta H^{n}_{i,j}\Delta\rho)^{2}} \left\{ K_{\rho_{i,j,k-\frac{1}{2}}} \left({}_{\ell}{}^{m}C^{*}_{i,j,k-1} + {}_{\ell}C^{n}_{i,j,k-1} \right) \right.$$

$$- \left(K_{\rho_{i,j,k-\frac{1}{2}}} + K_{\rho_{i,j,k+\frac{1}{2}}} \right) \left({}_{\ell}{}^{m}C^{*}_{i,j,k} + {}_{\ell}C^{n}_{i,j,k} \right)$$

$$\left. + K_{\rho_{i,j,k+\frac{1}{2}}} \left({}_{\ell}{}^{m}C^{*}_{i,j,k+1} + {}_{\ell}C^{n}_{i,j,k+1} \right) \right\} + \frac{1}{2} \left({}_{\ell}{}^{m}R^{*}_{i,j,k} + {}_{\ell}R^{n}_{i,j,k} \right) + {}_{\ell}S^{n+\frac{1}{2}}_{i,j,k} \qquad \text{(D-5)}$$

The boundary conditions are given by:

(1) $$\frac{-K_{\rho_{i,j,\frac{1}{2}}}}{\Delta H^{n}_{i,j}} \left(\frac{{}_{\ell}C^{n}_{i,j,1} - {}_{\ell}C^{n}_{i,j,0}}{\Delta\rho} \right) = {}_{\ell}Q^{n}_{i,j}$$

(2) if $W \geq 0$, then $${}_{\ell}C^{n}_{i,j,NOZ} = {}_{\ell}C^{n}_{i,j,NOZ+1}$$

$$\text{if } W < 0, \text{ then} \qquad {}_{\ell}g^{n}_{i,j,NOZ+\frac{1}{2}} = \frac{W}{2}\left({}_{\ell}C^{n}_{i,j,NOZ} + {}_{\ell}C^{n}_{i,j,NOZ+1}\right)$$

$$- \frac{K\rho_{i,j,NOZ+\frac{1}{2}}}{\Delta H^{n}_{i,j}\,\Delta\rho}\left({}_{\ell}C^{n}_{i,j,NOZ+1} - {}_{\ell}C^{n}_{i,j,NOZ}\right)$$

where NOZ refers to the mesh point just under the inversion base.

Equations (D-5) must be solved simultaneously for reactive hydrocarbon, nitrogen dioxide, ozone, and nitric oxide. One possible scheme is the solution of the forty nonlinear equations (10 layers x 4 species) by Newton's method. To avoid this, however, we have chosen to write the terms

$${}_{\ell}R^{m*}_{i,j,k}$$

in such a way that each interation only involves the inversion of a tridiagonal matrix for each species--a significant calculational simplification. (See von Rosenberg (1969) for a description of Thomas' algorithm for the inversion of tridiagonal matrices). As an example, consider the term

$${}_{1}R^{m*}_{i,j,k}$$

where $\ell = 1$ refers to reactive hydrocarbon.

The rate of formation of hydrocarbon through chemical reaction is given by

$$\frac{d(RH)}{dt} = -k_9(RH)(O) - k_{10}(RH)(O_3) - k_{11}(RH)(OH\cdot)$$

which we write:

$${}_{1}R^{m*}_{i,j,k} = -k_9\,{}_{1}C^{m*}_{i,j,k}\,{}^{m-1}RAD1^{*}_{i,j,k} - k_{10}\,{}_{1}C^{m*}_{i,j,k}\,{}_{2}C^{m-1*}_{i,j,k}$$

$$-k_{11}\,{}_{1}C^{m*}_{i,j,k}\,{}^{m-1}RAD2^{*}_{i,j,k}$$

where $\ell = 2$ refers to O_3, RAD1 to atomic oxygen, and RAD2 to $OH\cdot$.

The only unknown in $^{m}_{l}R^{*}_{i,j,k}$ is $^{m}_{l}C^{*}_{i,j,k}$,

and thus each iterative calculation for reactive hydrocarbon, as with all other species, reduces to the inversion of a tridiagonal matrix. The iteration is started using the concentrations at the previous time step,

$$^{0}_{l}C^{*}_{i,j,k} = {}_{l}C^{n}_{i,j,k}$$

It is terminated when

$$\left| \frac{^{m+1}_{l}C^{*}_{i,j,k} - {}^{m}_{l}C^{*}_{i,j,k}}{^{m+1}_{l}C^{*}_{i,j,k}} \right| \leq \varepsilon$$

Step II - Integration in the ξ direction

Having established values of $_{l}C^{*}_{i,j,k}$ from Step I, we now employ a second-order method in conservative form (i.e. we write $\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x}$ as $\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} - c \frac{\partial u}{\partial x}$), as given by Crowley (1968), to advance $_{l}C^{*}_{i,j,k}$ to $_{l}C^{**}_{i,j,k}$.

$$_{l}C^{**}_{i,j,k} = {}_{l}C^{*}_{i,j,k} \left[1 + \frac{\Delta t}{(x_E - x_W)\Delta \xi} \left(u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k} \right) \right]$$

$$+ \frac{\Delta t}{(x_E - x_W)\Delta \xi} \left({}_{l}F^{*}_{i-\frac{1}{2},j,k} - {}_{l}F^{*}_{i+\frac{1}{2},j,k} \right) \qquad \text{(D-6)}$$

where

$$\frac{\Delta t}{(x_E - x_W)\Delta \xi} \, {}_{l}F^{*}_{i-\frac{1}{2},j,k} = \frac{\alpha_{i-\frac{1}{2},j,k}}{2} \left({}_{l}C^{*}_{i-1,j,k} + {}_{l}C^{*}_{i,j,k} \right)$$

$$- \frac{(\alpha_{i-\frac{1}{2},j,k})^2}{2} \left({}_{l}C^{*}_{i,j,k} - {}_{l}C^{*}_{i-1,j,k} \right)$$

$$\alpha_{i-\frac{1}{2},j,k} = \frac{u_{i-\frac{1}{2},j,k} \, \Delta t}{(x_E - x_W)\Delta \xi}$$

The boundary conditions are written as

$$\frac{\Delta t}{(x_E - x_W)\Delta\xi}\ {}^{\ell}F^{*}_{\frac{1}{2},j,k} = \frac{u_{\frac{1}{2},j,k}\ \Delta t}{(x_E - x_W)\Delta\xi}\ {}^{\ell}g^{*}_{\frac{1}{2},j,k}$$

for $u_{\frac{1}{2},j,k} > 0$

$$\frac{\Delta t}{(x_E - x_W)\Delta\xi}\ {}^{\ell}F^{*}_{NOX+\frac{1}{2},j,k} = \frac{u_{NOX+\frac{1}{2},j,k}\ \Delta t}{(x_E - x_W)\Delta\xi}\ {}^{\ell}g^{*}_{NOX+\frac{1}{2},j,k}$$

for $u_{NOX+\frac{1}{2},j,k} < 0$

where $NOX+\frac{1}{2}$ refers to the x_E boundary.

At points of outflow we use a one-sided difference approximation. In particular,

$${}^{\ell}C^{**}_{1,j,k} = \left({}^{\ell}C^{*}_{1,j+1,k} + {}^{\ell}C^{*}_{1,j-1,k}\right)/2$$

$$+ \frac{u_{1,j,k}\ \Delta t}{(x_E - x_W)\Delta\xi}\left[\left({}^{\ell}C^{*}_{1,j-1,k} + {}^{\ell}C^{*}_{1,j+1,k}\right)/2 - {}^{\ell}C^{*}_{2,j,k}\right]$$

for $u_{1,j,k} \leq 0$

$${}^{\ell}C^{**}_{NOX,j,k} = \left({}^{\ell}C^{*}_{NOX,j-1,k} + {}^{\ell}C^{*}_{NOX,j+1,k}\right)/2$$

$$+ \frac{u_{NOX,j,k}\ \Delta t}{(x_E - x_W)\Delta\xi}\left[{}^{\ell}C^{*}_{NOX-1,j,k} - \left({}^{\ell}C^{*}_{NOX,j-1,k} + {}^{\ell}C^{*}_{NOX,j+1,k}\right)/2\right]$$

for $u_{NOX,j,k} \geq 0$

It should be noted that in moving from node to node in the ξ direction, only

$$\frac{\Delta t}{(x_E - x_W)\Delta\xi}\ {}^{\ell}F^{*}_{i+\frac{1}{2},j,k}$$

need be calculated, since $\frac{\Delta t}{(x_E - x_W)\Delta\xi}\ \ell^{F^*}_{i-\frac{1}{2},j,k}$ is available from the previous calculation.

Step III - Integration in the η *direction*

The final step in the integration is analogous to Step II.

$$\ell^{C^{n+1}}_{i,j,k} = \ell^{C^{**}}_{i,j,k}\left[1 + \frac{\Delta t}{(y_N - y_S)\Delta\eta}\left(v_{i,j+\frac{1}{2},k} - v_{i,j-\frac{1}{2},k}\right)\right]$$

$$+ \frac{\Delta t}{(y_N - y_S)\Delta\eta}\left(\ell^{G^{**}}_{i,j-\frac{1}{2},k} - \ell^{G^{**}}_{i,j+\frac{1}{2},k}\right)$$

where

$$\frac{\Delta t}{(y_N - y_S)\Delta\eta}\ \ell^{G^{**}}_{i,j-\frac{1}{2},k} = \frac{\beta_{i,j-\frac{1}{2},k}}{2}\left(\ell^{C^{**}}_{i,j-1,k} + \ell^{C^{**}}_{i,j,k}\right)$$

$$- \frac{(\beta_{i,j-\frac{1}{2},k})^2}{2}\left(\ell^{C^{**}}_{i,j,k} - \ell^{C^{**}}_{i,j-1,k}\right)$$

$$\beta_{i,j-\frac{1}{2},k} = \frac{v_{i,j-\frac{1}{2},k}\,\Delta t}{(y_N - y_S)\Delta\eta}$$

The boundary conditions are also treated in a manner analogous to Step II.

We now present the fourth-order approximation as given by Fromm (1969). Steps II' and III', in ξ and η respectively, are as follows:

Step II'. Integration in the ξ *direction*

We advance $\ell^{C^{*}}_{i,j,k}$ to $\ell^{C^{**}}_{i,j,k}$ by:

$$\ell^{C^{**}}_{i,j,k} = \ell^{C^{*}}_{i,j,k}\left\{1 + \frac{\Delta t}{24\,(x_E - x_W)}\left[27\left(u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k}\right)\right.\right.$$

$$\left.\left. - \left(u_{i+3/2,j,k} - u_{i-3/2,j,k}\right)\right]\right\}$$

$$+ \frac{\Delta t}{(x_E - x_W)\Delta\xi}\left(\ell^{(4)F^{*}}_{i-\frac{1}{2},j,k} - \ell^{(4)F^{*}}_{i+\frac{1}{2},j,k}\right)$$

where the left superscript (4) refers to the fourth-order difference operator given by

$$\frac{\Delta t}{(x_E - x_W)\Delta\xi}\ {}^{(4)}F^{*}_{i-\frac{1}{2},j,k} = \frac{\alpha_{i-\frac{1}{2},j,k}}{12}\left\{7\left({}^{\ell}C^{*}_{i-1,j,k} + {}^{\ell}C^{*}_{i,j,k}\right) - \left({}^{\ell}C^{*}_{i-2,j,k} + {}^{\ell}C^{*}_{i+1,j,k}\right)\right\}$$

$$+\frac{(\alpha_{i-\frac{1}{2},j,k})^2}{24}\left\{15\left({}^{\ell}C^{*}_{i-1,j,k} - {}^{\ell}C^{*}_{i,j,k}\right) - \left({}^{\ell}C^{*}_{i-2,j,k} - {}^{\ell}C^{*}_{i+1,j,k}\right)\right\}$$

$$+\frac{(\alpha_{i-\frac{1}{2},j,k})^3}{12}\left\{-\left({}^{\ell}C^{*}_{i-1,j,k} + {}^{\ell}C^{*}_{i,j,k}\right) + \left({}^{\ell}C^{*}_{i-2,j,k} + {}^{\ell}C^{*}_{i+1,j,k}\right)\right\}$$

$$+\frac{(\alpha_{i-\frac{1}{2},j,k})^4}{24}\left\{-3\left({}^{\ell}C^{*}_{i-1,j,k} - {}^{\ell}C^{*}_{i,j,k}\right) + \left({}^{\ell}C^{*}_{i-2,j,k} - {}^{\ell}C^{*}_{i+1,j,k}\right)\right\}$$

where

$$\alpha_{i-\frac{1}{2},j,k} = \frac{u_{i-\frac{1}{2},j,k}\Delta t}{(x_E - x_W)\Delta\xi}$$

For mesh points adjacent to the boundary, we use the second-order scheme given in Equation (D-6). The boundary conditions are the same as those presented in the second-order treatment of Step II.

Step III'. Integration in the η direction

We advance ${}^{\ell}C^{**}_{i,j,k}$ to ${}^{\ell}C^{n+1}_{i,j,k}$ by the η direction counterpart of Step II'.

$$
{}^{\ell}C^{n+1}_{i,j,k} = {}^{\ell}C^{**}_{i,j,k}\left\{1 + \frac{\Delta t}{24(y_N - y_S)\Delta\eta}\left[27\left(v_{i,j+\frac{1}{2},k} - v_{i,j-\frac{1}{2},k}\right)\right.\right.
$$

$$
\left.\left. - \left(v_{i,j+3/2,k} - v_{i,j-3/2,k}\right)\right]\right\}
$$

$$
+ \frac{\Delta t}{(y_N - y_S)\Delta\eta}\left({}^{(4)}_{\ell}G^{**}_{i,j-\frac{1}{2},k} - {}^{(4)}_{\ell}G^{**}_{i,j+\frac{1}{2},k}\right)
$$

where
$$
\frac{\Delta t}{(y_N - y_S)\Delta\eta}\,{}^{(4)}_{\ell}G^{**}_{i,j-\frac{1}{2},k} = \frac{\beta_{i,j-\frac{1}{2},k}}{12}\left\{7\left({}^{\ell}C^{**}_{i,j-1,k} + {}^{\ell}C^{**}_{i,j,k}\right)\right.
$$

$$
\left. -\left({}^{\ell}C^{**}_{i,j-2,k} + {}^{\ell}C^{**}_{i,j+1,k}\right)\right\}
$$

$$
+ \frac{\left(\beta_{i,j-\frac{1}{2},k}\right)^2}{24}\left\{15\left({}^{\ell}C^{**}_{i,j-1,k} - {}^{\ell}C^{**}_{i,j,k}\right)\right.
$$

$$
\left. -\left({}^{\ell}C^{**}_{i,j-2,k} - {}^{\ell}C^{**}_{i,j+1,k}\right)\right\}
$$

$$
+ \frac{\left(\beta_{i,j-\frac{1}{2},k}\right)^3}{12}\left\{-\left({}^{\ell}C^{**}_{i,j-1,k} + {}^{\ell}C^{**}_{i,j,k}\right)\right.
$$

$$
\left. +\left({}^{\ell}C^{**}_{i,j-2,k} + {}^{\ell}C^{**}_{i,j+1,k}\right)\right\}
$$

$$
+ \frac{\left(\beta_{i,j-\frac{1}{2},k}\right)^4}{24}\left\{-3\left({}^{\ell}C^{**}_{i,j-1,k} - {}^{\ell}C^{**}_{i,j,k}\right)\right.
$$

$$
\left. +\left({}^{\ell}C^{**}_{i,j-2,k} - {}^{\ell}C^{**}_{i,j+1,k}\right)\right\}
$$

The boundary conditions are treated in a manner analogous to Step II'.

III. EVALUATION AND DISCUSSION OF THE NUMERICAL METHOD

As was pointed out in Section I, alternative finite difference methods may be evaluated on the basis of stability, accuracy, and computing time and storage requirements. These characteristics have been examined as they pertain to the use of the method of fractional steps in the solution of Equations (D-4). We present our findings in the discussion that follows.

A. Stability

A theoretical stability analysis is a difficult undertaking for nonlinear equations or systems of equations. As Equations (D-4) are nonlinear, stability considerations were examined in two sequential steps:

1) Set $R_i = S_i = 0$ in Equations (D-4). Examine the stability of the resulting linear equations.

2) Examine the stability of the full Equations (D-4) through numerical experimentation.

Thus, a range of acceptable step sizes is estimated in Step 1. Step 2 is obviously necessary to assess the effect of the nonlinear terms on stability. While this approach does not ensure that stability problems will not be encountered over certain ranges of the independent variables--as the range studied in numerical experimentation is necessarily limited--it will provide a good indication as to whether problems of instability are likely.

We turn now to the application of the method of fractional steps to Equations (D-4). In integrating forward in time from

$$\ell C^{n}_{i,j,k} \quad \text{to} \quad \ell C^{n+1}_{i,j,k}$$

stability is assured if each fractional step is stable. Thus, we must examine the stability of the numerical procedures that constitute each of the three steps.

Step I is basically the solution of the equation

$$\frac{\partial c_i}{\partial t} + \frac{W}{\Delta H}\frac{\partial c_i}{\partial \rho} = \frac{1}{\Delta H^2}\frac{\partial}{\partial \rho}\left(K_\rho \frac{\partial c_i}{\partial \rho}\right) + R_i + S_i$$

Since this equation is nonlinear, we first set $R_i = S_i = 0$. The procedure commonly applied to the solution of the resulting linear equation, the Crank-Nicolson finite difference scheme, is stable for all values of Δt. We must rely on numerical experiments to ascertain if the reaction and source terms give rise to

instability over the range of step sizes (in time) of interest--on the order of one to five minutes. In preliminary studies, no evidence of instability has been observed. We plan to carry out additional tests of the accuracy of numerical techniques in the future; these same tests will be useful in further assessing stability.

Step II is represented by the numerical integration of

$$\frac{\partial c_i}{\partial t} + \left(\frac{u}{x_E - x_W}\right) \frac{\partial c_i}{\partial \xi} = 0$$

Crowley (1968) has shown that a condition for stability is that $|\alpha|<1$, where

$$\alpha = \frac{u\Delta t}{(x_E - x_W)\Delta \xi} \quad .$$

Our experience thus far has indicated that α is usually less than 0.1. Step III, in the η direction, is the direct counterpart of Step II, in that $|\beta|<1$, is the condition for stability, where

$$\beta = \frac{v\Delta t}{(y_N - y_S)\Delta \eta}$$

No evidence of instability has been observed when these conditions were satisfied.

B. Accuracy

While the goal of model validation is to obtain reasonable quantitative agreement between predicted and observed pollutant concentrations, validation runs cannot serve as a basis for evaluating the accuracy of the numerical technique, as discrepancies are attributable not only to truncation errors, but also to possible inadequacies of the model and inaccuracies in the data. Further, as was the case with stability analysis, theoretical calculation of the magnitude of truncation errors is difficult due to the non-linearity of the model. Thus, we must again turn to test studies--first for the case in which nonlinear terms are neglected, and second through comparative studies of the full model.

The spatial truncation error may be reduced in two ways--by reducing the spatial interval between nodes (or, equivalently, by reducing the dimensions of a grid square) and by increasing the order of the numerical approximation. The horizontal spatial grid is presently comprised of 2 mile x 2 mile squares. The selection of this grid gives recognition to the fact that, even though this spacing is far too coarse to represent the transport processes with accuracy, meteorological data is too sparse to justify finer detail.

The effect of grid spacing on computational accuracy can be assessed, however, rather easily. One need only perform a validation run for a small portion of the Basin, using first the 2 mile x 2 mile grid, then a 1 mile x 1 mile grid. The differences observed in predicted values of concentrations give an indication of the magnitude of the truncation errors. While this test has not been carried out, it is planned for the beginning of the next phase of our studies.

The effect of the order of the method on accuracy has been assessed for a simplified form of the continuity equations,

$$\frac{\partial c}{\partial t} + \left(\frac{u}{x_E - x_W}\right)\frac{\partial c}{\partial \xi} + \left(\frac{v}{y_N - y_S}\right)\frac{\partial c}{\partial \eta} = 0 \qquad \text{(D-7)}$$

under conditions of uniform air flow. Following Crowley (1968), we first examined the effect of transporting a conical distribution of concentration across a 2 mile x 2 mile grid (see Figure D-1). The following conditions applied to the test:

Wind:	Uniform, $6\sqrt{2}$ mph, from the southwest (moving northeast at 45°) thus $u = 6$ mph, $v = 6$ mph
Grid Spacing:	$x_E - x_W = y_N - y_S = 50$ miles $\Delta x = \Delta y = 2$ miles (or $\Delta\xi = \Delta\eta = 0.04$)
Initial Concentration Distribution:	Right circular cone with concentration of 2 ppm at apex, 1 ppm at base, and 1 ppm at all other points (see Figure D-1)
Time Step:	10 minutes

The combination of wind speed and direction and size of the time step conspire to move the distribution exactly one-half a grid spacing per time step in both the ξ and η directions. In Table D-1, we report the errors in the peak concentration that accumulate over a five-hour period, the time required to traverse 60% of the Basin. Note that the fourth-order approximation, as applied to the numerical solution of Equation (D-7) proved to be substantially more accurate in predicting peak concentrations than the second-order method. Furthermore, using the fourth-order approximation, after one-hour all other predicted concentrations were accurate to within 2%, and after five hours, to within 4%.

In a second test, we investigated the effects of the same wind field on the 0500 PST carbon monoxide concentration distribution shown in Figure D-2. A fourth-order approximation was applied to Equation (D-7) in this test, with a time step of ten minutes. After

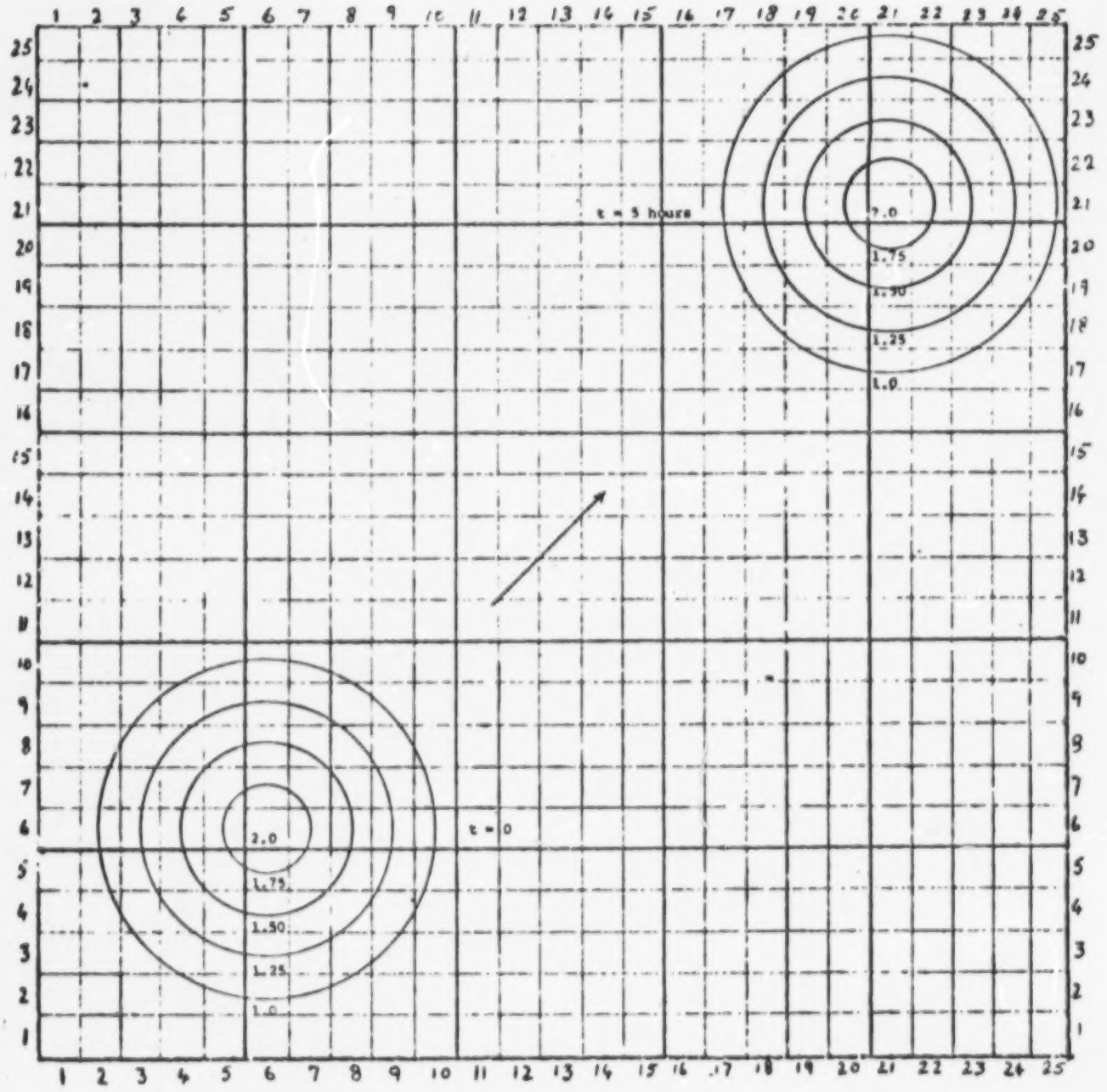

Figure D-1. TEST DISCRIPTION AND ITS PATH OF TRANSPORT

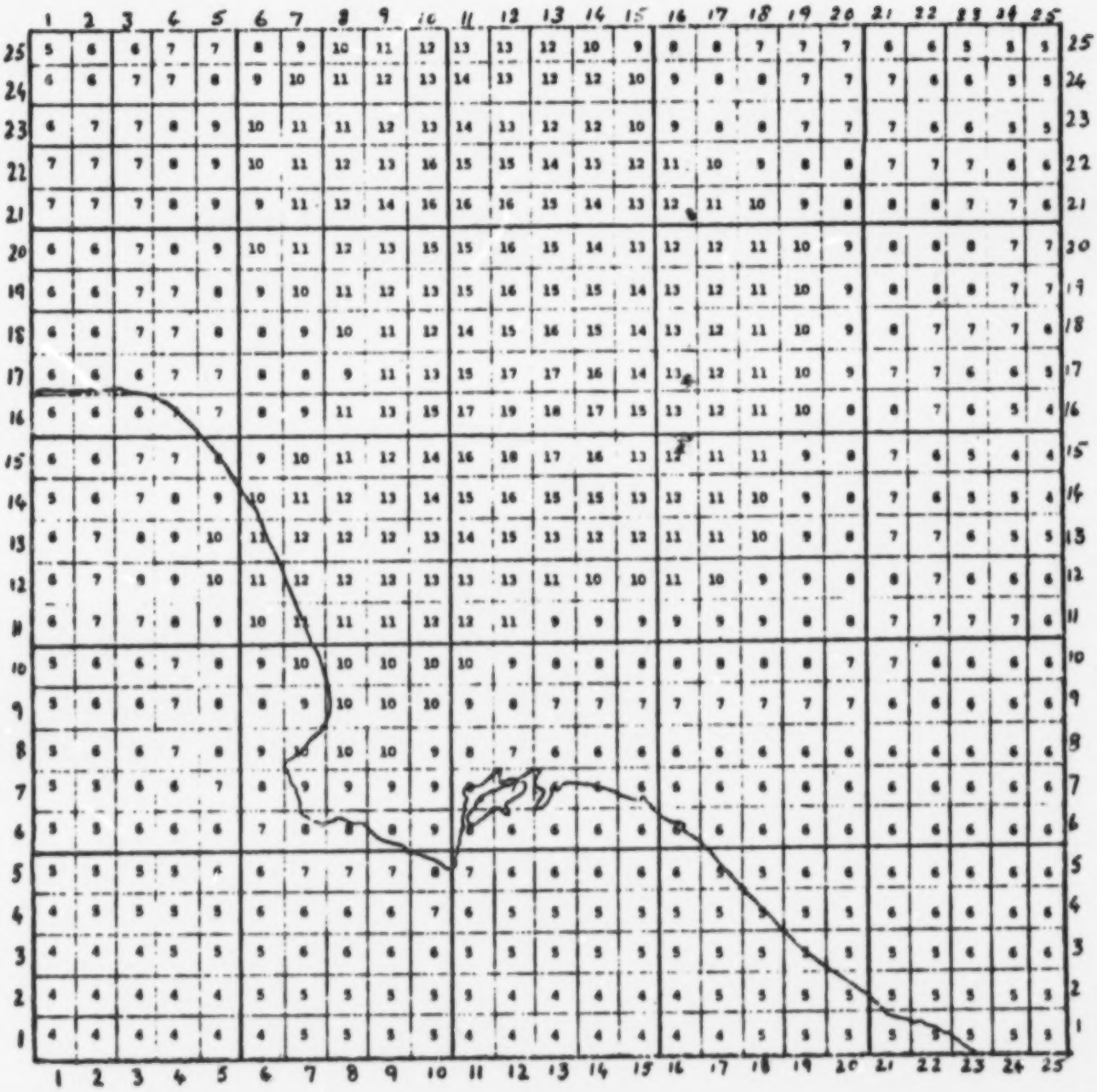

Figure D-2. CO CONCENTRATIONS, PPM. 30 September 1969, 500 PST (600 PDT)

TABLE D-1. RESULTS OF TESTS OF THE NUMERICAL TECHNIQUE

	Second Order		Fourth Order	
Time (hr.)	Peak Conc. (ppm)	Error (ppm)	Peak Conc.	Error
0	2.0	0.0	2.0	0.0
1	1.83	-0.17	1.87	-0.13
2	1.78	-0.22	1.86	-0.14
3	1.74	-0.26	1.86	-0.14
4	1.68	-0.32	1.85	-0.15
5	1.69	-0.31	1.84	-0.16

four hours, the maximum discrepancy between predicted and correct values of concentration was 1.5 ppm, with the vast majority accurate to less than 1 ppm.

While these tests confirm the accuracy of the fourth-order method of fractional steps as applied to horizontal convective transport (Equation (D-7)), the degree to which these results are reflective of the accuracy that can be expected when the method is applied to the full model is unknown. The nonuniformity of flow typical of the meteorology of Los Angeles, the effect of the nonlinear terms, the coupling with diffusion and advection in the vertical, the relatively smooth and even distribution of concentration that prevails over most of the Basin are all factors that affect accuracy. Also, it is unclear whether the greater accuracy of the fourth-order approximation in the horizontal (Steps II and III) is warranted when a second-order approximation is used for calculations in the vertical (Step I). In other words, the greater accuracy of the higher-order method may be forfeited when approximations of differing orders are applied in the same calculation. Thus, a number of questions remain unanswered with respect to the accuracy of the procedure.

In future studies, we plan to compare second and fourth-order methods for Steps II and III when applied to the full airshed model. If the differences in predicted values do not vary greatly, this may be an indication that either errors in the vertical calculations are of the order of those associated with the second-order approximation in the horizontal, or that nonuniform flow characteristics or the nonlinear terms serve to lessen the difference in accuracy between second and fourth-order methods. Conversely, if the differences in prediction are substantial, the fourth-order approximation will be adopted for use despite the added computing time that this method entails. In the validation studies reported in the main text, we have used the second-order method, feeling that this would prove sufficient for initial evaluation of the model's performance.

C. Computing Storage and Time Requirements

The full airshed model currently requires a storage capacity of 315,000 bytes. It may be possible to reduce the storage requirements in several ways:

1. Exclude a portion of the nodes lying over the ocean, for instance, those more than four miles from shore. This would result in a 15-25% reduction in nodes and thus a 20,000-40,000 byte reduction in storage. Computation time would also be reduced.

2. Reduce the number of grid points in the vertical direction from the present 10 to 5-7. Present results indicate that such a reduction would not have an appreciable effect on the accuracy of the calculation. However, specific tests are needed to substantiate this point.

3. Use peripheral storage and overlay portions of the program.

We will investigate each of these possibilities in future work.

As the computer program is currently constituted, two seconds of computation time (on an IBM 360-75) are required per time step for the prediction of carbon monoxide concentrations over a 25 x 25 x 10 grid. Thus, if Δt = 2 minutes, one minute of computation time is needed to simulate one hour of actual time. It should be mentioned that, while we are now using a two-minute time step in validation runs for carbon monoxide, a longer time step may well be adequate--perhaps on the order of five minutes. We plan to investigate the effect of variations in the length of time steps in the near future.

Preliminary tests of the model with all six species included indicate that for two-minute time steps the ratio of simulated time to computing time is approximately eight. Thus, an eight-hour simulation would require one hour of computation. However, more computing experience is needed with reactive species included in the model to better establish this ratio.

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